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DENSE HETEROGENEOUS CONTINUUM MODEL OF TWO-PHASE EXPLOSION FIELDS

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Abstract

A heterogeneous continuum model is proposed to describe the dispersion of a dense Aluminum particle cloud in an explosion. Let α_1 denote the volume fraction occupied by the gas and α_2 the fraction occupied by the solid, satisfying the volume conservation relation: $\alpha_1 + \alpha_2 = 1$. When the particle phase occupies a non-negligible volume fraction (i.e., $\alpha_2 > 0$), additional terms, proportional to α_2, appear in the conservation laws for two-phase flows. These include: (i) a particle pressure (due to particle collisions), (ii) a corresponding sound speed (which produces real eigenvalues for the particle phase system), (iii) an Archimedes force induced on the particle phase (by the gas pressure gradient), and (iv) multi-particle drag effects (which enhance the momentum coupling between phases). These effects modify the accelerations and energy distributions in the phases; we call this the Dense Heterogeneous Continuum Model. A characteristics analysis of the Model equations indicates that the system is hyperbolic with real eigenvalues for the gas phase: $\{\mathbf{v}_1, \mathbf{v}_1 \pm a_1\}$ and for the "particle gas" phase: $\{\mathbf{v}_2, \mathbf{v}_2 \pm a_2\}$ and the particles: $\{\mathbf{v}_2\}$, where $\mathbf{v}_i$ and a_i denote the velocity vector and sound speed of phase i. These can be used to construct a high-order Godunov scheme to integrate the conservation laws of a dense heterogeneous continuum.

1. Introduction

A dense heterogeneous continuum model is proposed to describe the initial stages of the dispersion of Aluminum (Al) particle clouds by a booster charge. This is an extension of a dilute heterogeneous continuum model we have used successfully to describe Al particle combustion in Shock-Dispersed-Fuel (SDF) explosions [1, 2].

We start by defining the volume fraction, $\alpha_i \equiv v_i / V$, of the volume V occupied by the gas (subscript 1) and particle phase (subscript 2). They satisfy the volume conservation relation:

$$\alpha_1 + \alpha_2 = 1 \tag{1}$$

According to Nigmatulin [3], when the particle phase occupies a non-negligible volume fraction (i.e., $\alpha_2 > 0$), additional terms appear in the conservation laws of two-phase flows:

- A particle pressure: $p_2(\alpha_2)$ due to particle collisions
- A sound speed: $a_2(\alpha_2)$ which produces real eigen-values for the particle phase system
- An Archimedes force: $\alpha_2 \nabla p_1$ induced on the particle phase by the gas pressure gradient
- And multi-particle drag coefficient: $C_D(\mathrm{Re}, \alpha_2)$, enhancing coupling between phases

These effects modify the accelerations and energy distributions in the phases; we call this the dense heterogeneous continuum model. The formulation of the model is described in §2. The conservation laws governing a dense heterogeneous continuum are presented in §3; this is followed by inter-phase interaction modes in §4. A summary of the characteristics analysis of this two-phase hyperbolic system is presented in §5. This is followed by conclusions in §6. For convenience of the reader, the notation is defined in Appendix A. More details of the characteristics analysis is presented in Appendix B.

2. Formulation

We assume that the particle phase behaves as a dense heterogeneous continuum. We view it as a particle gas (analogous to a molecular gas) that, according to kinetic theory [4, 5], contains a particle pressure, p_2, temperature, T_2, and energy, e_2, due to particle collisions:

$$p_2 \equiv \frac{1}{3}\frac{m}{V}\overline{\left\langle C^2 \right\rangle} \tag{2}$$

$$T_2 = \frac{1}{3}\frac{m}{k}\overline{\left\langle C^2 \right\rangle} \tag{3}$$

$$e_2 = \frac{1}{2}\overline{\left\langle C^2 \right\rangle} \tag{4}$$

These depend on the mean kinetic energy of the particles $\overline{\left\langle C^2 \right\rangle}$, where C denotes the particle speed, m its mass while V is volume. Based on Nigmatulin [3], we model the particle pressure by the compaction pressure relation:

$$p_2(\alpha_2) = p_{2,0}\left(\frac{\alpha_2}{\alpha_2^* - \alpha_2}\right)^{\chi} \tag{5}$$

where $\alpha_2^* \sim 0.5$ and $\chi = 5/3$ (hard sphere model). Then we define the energy of the particle phase from the First Law of Thermodynamics applied to this adiabatic system:

$$de_2 = -p_2 dV \tag{6}$$

In addition, particles can store energy, e_s, due to the thermal heat capacity of the solid:

$$e_s(T_s) = c_{v,s} T_s \tag{7}$$

where T_s is the temperature of the solid particle and $c_{v,s}$ is its specific heat. Once could call this a 2-temperature model of the particle phase. How these terms affect the momentum and energy balance of the two-phase flow is described in the next section.

3. Conservation Laws

3.1 Mass Conservation

We assume that the density of the gas and particle phases may be described by Eulerian continuum functions: $\rho_1(\mathbf{x},t)$, and $\rho_2(\mathbf{x},t)$. Their evolution per unit volume, is specified by the following mass conservation laws:

- gas phase: $\partial_t\rho_1 + \nabla\rho_1\mathbf{v}_1 = j_{21}$ (8)
- particle phase: $\partial_t\rho_2 + \nabla\rho_2\mathbf{v}_2 = -j_{21}$ (9)
- mixture: $\partial_t\rho_m + \nabla\rho_m\mathbf{v}_m = 0$ (10)

where the mixture density is $\rho_m \equiv \rho_1 + \rho_2$. The source term: j_{21} represents the mass exchange from the particle phase to the gas phase; a model of this mass interchange is specified in §4. The third relation (10) shows that, according to the formulation, the two-phase mixture conserves mass. The volume fraction of the particle phase, which will be needed in subsequent relations, is determined from the definition:

$$\alpha_2 \equiv \rho_2/\rho_2^0 \tag{11}$$

3.2 Momentum Conservation

We assume that the momentum of the gas and particle phases may be described by Eulerian continuum functions: $\rho_1(\mathbf{x},t)\mathbf{v}_1(\mathbf{x},t)$ and $\rho_2(\mathbf{x},t)\mathbf{v}_2(\mathbf{x},t)$. Their evolution per unit volume, is specified by the following momentum conservation laws:

- gas phase: $\partial_t\rho_1\mathbf{v}_1 + \nabla(\rho_1\mathbf{v}_1\mathbf{v}_1 + p_1) = -\alpha_1\dot{\mathbf{f}}_s + j_{21}\mathbf{v}_2$ (12)
- particle phase: $\partial_t\rho_2\mathbf{v}_2 + \nabla(\rho_2\mathbf{v}_2\mathbf{v}_2 + p_2 + \alpha_2 p_1) = \alpha_1\dot{\mathbf{f}}_s - j_{21}\mathbf{v}_2$ (13)
- mixture: $\partial_t\rho_m\mathbf{v}_m + \nabla(\rho_m\mathbf{v}_m\mathbf{v}_m + p_m + \alpha_2 p_1) = 0$ (14)

where the mixture momentum and pressure are defined by the relations $\rho_m\mathbf{v}_m \equiv \rho_1\mathbf{v}_1 + \rho_2\mathbf{v}_2$ and $p_m \equiv p_1 + p_2$, respectively. For the gas phase, the pressure is determined from the perfect gas relation:

$$p_1 \equiv \alpha_1 p_1^0 = \rho_1 R_1 T_1 \tag{15}$$

along with the equation of state relation: $T_1 = u_1^{-1}(T_1)$. The source term: $\dot{\mathbf{f}}_s$ represents the drag force which accelerates the particle phase and depletes momentum from the gas phase. The source term: $j_{21}\mathbf{v}_2$ represents the rate of momentum change induced by the mass exchange j_{21}. Note in eq. (13), that the particle phase momentum is influenced by gradient of the particle pressure: ∇p_2, and by the gradient in the gas pressure (the so-called Archimedes force): $\nabla\alpha_2 p_1$; here α_2 represents the particle cross-sectional area loaded by the gas force. Being proportional to α_2, both these forces are absent in dilute heterogeneous systems (where $\alpha_2 = 0$). The third relation (3.8) shows that, according to the formulation, the two-phase mixture conserves momentum.

3.3 Energy Conservation

We assume that the energy of the phases may be described by Eulerian continuum functions for the gas phase: $\rho_1(\mathbf{x},t)\,u_1(\mathbf{x},t)$, and for the particle phase: $\rho_2(\mathbf{x},t)\,e_2(\mathbf{x},t)$ and $\rho_2(\mathbf{x},t)\,e_s(\mathbf{x},t)$. The evolution of the gas phase is specified by:

- gas phase: $$\partial_t \rho_1 E_1 + \nabla\cdot(\rho_1 \mathbf{v}_1 E_1 + p_1 \mathbf{v}_1) = -\dot{q}_s - \dot{\mathbf{f}}_s\cdot\mathbf{v}_1 + j_{21}E_2 \tag{16}$$

where $E_1 = u_1(T_1) + \mathrm{v}_1^2/2$ denotes the total energy of the gas. It can loose energy by heat transfer to the solid particles: $\dot{q}_s$ and by drag work: $\dot{\mathbf{f}}_s\cdot\mathbf{v}_1$; and gain energy due to mass transfer: $j_{21}E_2$ from the solid phase.

The evolution of the particle internal energy (IE), kinetic energy (KE), and thermal energy (TE) obey the following:

- particle IE: $$\partial_t \rho_2 e_2 + \nabla\cdot(\rho_2\mathbf{v}_2 e_2) + (p_2 + \alpha_2 p_1)\nabla\cdot\mathbf{v}_2 = 0 \tag{17}$$
- particle KE: $$\partial_t \rho_2 \mathrm{v}_2^2/2 + \nabla\rho_2\mathbf{v}_2\mathrm{v}_2^2/2 + \mathbf{v}_2\cdot\nabla(p_2+\alpha_2 p_1) = \mathbf{v}_2\cdot\alpha_1\dot{\mathbf{f}}_s - j_{21}\,\mathrm{v}_2^2 \tag{18}$$
- particle TE: $$\partial_t \rho_2 e_s + \nabla\cdot(\rho_2\mathbf{v}_2 e_s) = \dot{q}_s - j_{21}e_s \tag{19}$$

The first represents a statement of the First Law of Thermodynamics, where the effective pressure: $p_2 + \alpha_2 p_1$ does work to change the particle internal energy. The second represents a dot product of particle momentum equation (3.7) with $\mathbf{v}_2$. The third represents heating of the solid particles by heat transfer from the gas: $\dot{q}_s$, and losses due to mass transfer: $j_{21}e_s$. A total energy equation of the particle phase, based on the definition: $E_2 = e_2(\alpha_2) + \mathrm{v}_2^2/2$, may be constructed by adding the IE and KE equations, yielding:

- Total: $$\partial_t \rho_2 E_2 + \nabla\cdot(\rho_2\mathbf{v}_2 E_2 + \{p_2 + \alpha_2 p_1\}\mathbf{v}_2) = \dot{f}_s\cdot\mathbf{v}_1 - j_{21}E_2 \tag{20}$$

This is analogous to the total energy conservation for the gas (3.11), and may be expected to have somewhat similar properties. Continuing along this same vein, one can construct a total energy conservation equation for the mixture: $\rho_m E_m \equiv \rho_1 E_1 + \rho_2 E_2 + \rho_2 e_s$, yielding:

- Mixture: $$\partial_t \rho_m E_m + \nabla\cdot(\rho_m \mathbf{v}_m E_m + p_m \mathbf{v}_m) = 0 \tag{21}$$

where the mixture pressure is defined by $p_m \mathbf{v}_m \equiv p_1 \mathbf{v}_1 + p_2 \mathbf{v}_2 + \alpha_2 p_1 \mathbf{v}_2$. This shows that, according to the formulation, the two-phase mixture conserves energy.

4. Inter-phase Exchanges

Mass Interchange (*from particle phase to gas phase*)

- particle $$j_{21} = \begin{cases} 0 & T_s < T_L \\ 3\sigma(1 + 0.276\sqrt{Re_s})/t_s & T_s \geq T_L \end{cases} \quad \text{where} \quad t_s = K d_s^2 \tag{22}$$

Momentum Interchange:

- drag force: $$\dot{\mathbf{f}}_s = C_D(\mathrm{Re}, \alpha_2) \cdot (\pi a^2 \rho_1^0 w_{12}^2 / 2) \mathbf{w}_{12} / w_{12} \quad \text{where} \quad \mathbf{w}_{12} \equiv \mathbf{v}_1 - \mathbf{v}_2 \tag{23}$$
- single particle: $$C_\mu^0(\mathrm{Re}) = \frac{24}{\mathrm{Re}_{12}} + \frac{4.4}{\sqrt{\mathrm{Re}_{12}}} + 0.42 \quad \text{where} \quad \mathrm{Re}_{12} = \rho_1^0 |\mathbf{v}_1 - \mathbf{v}_2| / \mu_1 \tag{24}$$
- multi-particle: $$C_D(\mathrm{Re}, \alpha_2) = C_\mu^0(\mathrm{Re}) \cdot \psi_\alpha(\alpha_2) \tag{25}$$
- porosity: $$\psi_\alpha(\alpha_2) = [1 - \alpha_2]^{-m} \quad \text{where} \quad m \cong \begin{cases} 5 & (\mathrm{Re} < 1) \\ 2.7 & (\mathrm{Re} > 1) \end{cases} \tag{26}$$

Energy Interchange:

- Heat Exchange: $$\dot{q}_s = \frac{6\sigma}{\rho_s d_s} \left[\frac{Nu \lambda_1 (T_1 - T_2)}{d_s} + \varepsilon \sigma_{Boltz} (T_1^4 - T_2^4) \right] \tag{27}$$
- Nusselt Number: $$Nu = 2 + 0.6 \mathrm{Pr}_1 \sqrt{\mathrm{Re}_{12}} \quad \& \quad Pr_1 = C_{p1} \mu_1 / k_1 \tag{28}$$

Particle Volume Effects on Drag Law

- dilute: $$C_\mu^{(1)}(\mathrm{Re}_{12}) = \frac{24}{\mathrm{Re}_{12}} + \frac{4.4}{\sqrt{\mathrm{Re}_{12}}} + 0.42 \qquad \alpha_2 \leq 0.08 \tag{29}$$
- dense: $$C_\mu^{(2)}(\mathrm{Re}_{12}, \alpha_i) = \frac{4}{3\alpha_1} \left[1.75 + \frac{150\alpha_2}{\alpha_1 \mathrm{Re}_{12}} \right] \qquad 0.45 \leq \alpha_2 < \alpha_2^* \tag{30}$$
- blend: $$C_\mu^0(\mathrm{Re}_{12}, \alpha_i) = \frac{(\alpha_2 - .08) C_\mu^{(2)} + (0.45 - \alpha_2) C_\mu^{(1)}}{0.37} \qquad 0.08 \leq \alpha_2 \leq 0.45 \tag{31}$$

5. Characteristics

A characteristics analysis [5] of the Dense Heterogeneous Continuum Model equations: (8)—(21) has been performed; an overview is outlined in Appendix B. Results of the analysis indicate that the Model equations are hyperbolic, with real wave speeds for both the gas and particle phases:

- gas: $$\mathbf{v}_1, \mathbf{v}_1 \pm a_1 \tag{32}$$
- "particle gas": $$\mathbf{v}_2, \mathbf{v}_2 \pm a_2 \tag{33}$$
- particle: $$\mathbf{v}_2 \tag{34}$$

along with corresponding sound speeds

- gas: $$a_1 = \sqrt{\frac{\gamma_1 p_1}{\rho_1}} \tag{35}$$
- particle gas: $$a_2 = \sqrt{\frac{1}{\rho_2^0}\left(\frac{\partial p_2}{\partial \alpha_2} + p_1\right)} \tag{36}$$

These can be used to construct a high-order Godunov scheme to integrate the conservation laws for a dense heterogeneous continuum.

6. Conclusions

When one considers a finite volume of the particle phase ($\alpha_2 > 0$), additional terms appear in the momentum and energy equations of two-phase flow, for example: particle pressure (and its corresponding sound speed), an Archimedes force, and multi-particle drag effects. We call this the Dense Heterogeneous Continuum Model. Characteristics analysis shows that this Model is hyperbolic, with real eigenvalues for the gas phase: $\{\mathbf{v}_1, \mathbf{v}_1 \pm a_1\}$ and for the "particle gas" phase: $\{\mathbf{v}_2, \mathbf{v}_2 \pm a_2\}$ and the particles: $\{\mathbf{v}_2\}$. These can be used to construct a high-order Godunov scheme to integrate the conservation laws of a dense heterogeneous continuum. Such effects are expected to be important during the particle dispersion phase of SDF explosions, and we intend to explore the influence of these forces in future numerical simulations.

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Appendix A: Notation

1. Volume (cc)

- gas: v_1 (A.1a)
- particle: v_2 (A.1b)
- mixture: $v_1 + v_2 = V$ (A.1c)

2. Volume Fraction

- gas: $\alpha_1 = v_1 / V$ (A.2a)
- particle: $\alpha_2 = v_2 / V \qquad 0 \le \alpha_2 < \alpha_2^* \;\;\&\;\; \alpha_2^* \sim 0.5$ (A.2b)
- conservation: $\alpha_1 + \alpha_2 = 1$ (A.2c)

3. True Density (g/cc)

- gas: $\rho_1^0 = m_1 / v_1$ (A.3a)
- particle: $\rho_2^0 = m_2 / v_2 \quad$ (solid density, constant) (A.3b)

4. Apparent Density (g/cc)

- gas: $\rho_1 = \dfrac{m_1}{V} = \dfrac{m_1}{v_1}\dfrac{v_1}{V} = \rho_1^0 \alpha_1 \quad$ where $\quad \alpha_1 = 1 - \alpha_2$ (A.4a)
- particle: $\rho_2 = \dfrac{m_2}{V} = \dfrac{m_2}{v_2}\dfrac{v_2}{V} = \rho_2^0 \alpha_2 \qquad \therefore \qquad \boxed{\alpha_2 \equiv \rho_2 / \rho_2^0}$ (A.4b)
- mixture: $\rho_m = \dfrac{m_1 + m_2}{V} = \rho_1 + \rho_2$ (A.4c)

5. True Pressure (in volume v_1)

- gas: $p_1^0 = \rho_1^0 R_1 T_1 = \dfrac{1}{\alpha_1} \rho_1 R_1 T_1$ (A.5a)

6. Apparent Pressure (in volume *V*)

- gas: $p_1 \equiv \alpha_1 p_1^0 = \rho_1 R_1 T_1$ (A.6a)
- particle: $p_2(\alpha_2) = p_{2,0} \left(\dfrac{\alpha_2}{\alpha_2^* - \alpha_2} \right)^{\chi}$ where $\; 0 < \chi < 2 \;\;\&\;\; \alpha_2^* \sim 0.5$ (A.6b)

7. Sound Speed (in volume *V*)

- gas: $a_1^2(T_1) \equiv \left(\dfrac{\partial p_1}{\partial \rho_1} \right)_s = \gamma_1 \dfrac{p_1}{\rho_1} = \gamma_1 R_1 T_1$ (A.7a)
- particle: $a_2^2(\alpha_2) \equiv \left(\dfrac{\partial p_2}{\partial \rho} \right)_s = \dfrac{1}{\rho_2^0} \left(\dfrac{\partial p_2}{\partial \alpha_2} + p_1 \right)$ (A.7b)

8. Specific Internal Energy (per unit mass)

- gas: $u_1(T) = a_1 T_1^2 + b_1 T_1 + c_1$ (A.8a)
- particle: $e_2 = -\int p_2 dv_2$ (A.8b)
- solid: $e_s = c_{\mathrm{v},s} T_s$ (A.8b)

9. Temperature

- gas: $T_1 = [-b_1 + \sqrt{b_1^2 - 4a_1(c_1 - u_1)}]/2a_1$ (A.9a)
- particle: $T_2 = f(\alpha_2)$ (A.9b)
- solid: $T_s = e_s / c_{\mathrm{v},s}$ (A.9c)

Appendix B: Characteristic Analysis [6]

Linearized Conservation Laws: $\mathrm{U}_t + \mathbf{A}U_x = 0$ (B.1)

$$\mathrm{U} = \begin{pmatrix} \rho_1 \\ \mathrm{v}_1 \\ T_1 \\ \rho_2 \\ \mathrm{v}_2 \\ e_2 \\ e_s \end{pmatrix}, \quad \mathbf{A} = \begin{pmatrix} \mathrm{v}_1 & \rho_1 & 0 & & & & \\ \frac{RT_1}{\rho_1} & \mathrm{v}_1 & R & & & & \\ 0 & \frac{RT_1}{c_{\mathrm{v}1}} & \mathrm{v}_1 & & & & \\ \frac{\alpha_2 RT_1}{\rho_2} & 0 & \frac{\alpha_2\rho_1 R}{\rho_2} & \mathrm{v}_2 & \rho_2 & 0 & 0 \\ & & & \frac{1}{\rho_2\rho_s}\left(\frac{\partial p_2}{\partial \alpha_2} + p_1\right) & \mathrm{v}_2 & 0 & 0 \\ & & & 0 & \frac{p_2+\alpha_2 p_1}{\rho_s} & \mathrm{v}_2 & 0 \\ & & & 0 & 0 & 0 & \mathrm{v}_2 \end{pmatrix} \tag{B.2}$$

The system is hyperbolic if **A** is diagonalizable with real eigenvalues, so that we can decompose **A** according to:

$$\mathbf{A} = \mathrm{R}\,\Lambda\,\mathrm{R}^{-1} \tag{B.3}$$

$$\mathrm{R}^{-1}\mathbf{A}\,\mathrm{R} = \Lambda \tag{B.4}$$

Eigenvalues:

$$\Lambda = \begin{pmatrix} \mathrm{v}_1 & & & & & & \\ & \mathrm{v}_1 + a_1 & & & & & \\ & & \mathrm{v}_1 - a_1 & & & & \\ & & & \mathrm{v}_2 & & & \\ & & & & \mathrm{v}_2 + a_2 & & \\ & & & & & \mathrm{v}_2 - a_2 & \\ & & & & & & \mathrm{v}_2 \end{pmatrix} \tag{B.5}$$

Wave Speeds

- gas: $\mathbf{v}_1, \mathbf{v}_1 \pm a_1$ (B.6)
- "particle gas": $\mathbf{v}_2, \mathbf{v}_2 \pm a_2$ (B.7)
- particle: $\mathbf{v}_2$ (B.8)

Sound Speeds

- gas: $a_1 = \sqrt{\dfrac{\gamma_1 p_1}{\rho_1}}$ (B.9)
- particle gas: $a_2 = \sqrt{\dfrac{1}{\rho_2^0}\left(\dfrac{\partial p_2}{\partial \alpha_2} + p_1\right)}$ (B.10)